## GC-Bench: An Open and Unified Benchmark for **Graph Condensation**

## Appendix

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#### C Reproducibility and Limitations 29

Submitted to the 38th Conference on Neural Information Processing Systems (NeurIPS 2024) Track on Datasets and Benchmarks. Do not distribute.

## 30 A Details of GC-Bench

### 31 A.1 Datasets

32 The evaluation node-level datasets include 5 homogeneous datasets (3 transductive datasets, i.e.,

33 Cora, Citeseer [14] and ogbn-arxiv [11], and 2 inductive datasets, i.e., Flickr [38] and Reddit [10])

and 2 heterogeneous datasets (ACM [41] and DBLP [6]). The evaluation graph-level datasets include

<sup>35</sup> 5 datasets (*NCII* [29], *DD* [3], *ogbg-molbace* [11], *ogbg-molbiv* [11], *ogbg-molbbbp* [11]).

<sup>36</sup> We utilize the standard data splits provided by PyTorch Geometric [5] and the Open Graph Benchmark

 $_{37}$  (OGB) [11] for our experiments. For datasets in TUDataset [25], we split the data into 10% for

testing, 10% for validation, and 80% for training. For ACM and DBLP datasets, we follow the settings

<sup>39</sup> outlined in [23]. Dataset statistics are shown in Table A1.

Table A1: Dataset statistics. For heterogeneous datasets, the features are from the target nodes (papers in *ACM* and authors in *DBLP*).

	Dataset	#Nodes / #Avg. Nodes	#Edges / #Avg. Edges	#Classes	#Features / Graphs
	Cora	2,708	5,429	7	1,433
T	Citeseer	3,327	4,732	6	3,703
eve	ogbn-arxiv	169,343	1,166,243	40	128
Ŀ	Flickr	89,250	899,756	7	500
po	Reddit	232,965	57,307,946	210	602
$\mathbf{Z}$	ACM	10,942	547,872	3	1,902
	DBLP	37,791	170,794	4	334
el	ogbg-molhiv	25.5	54.9	2	41,127
lev	ogbg-molbace	34.1	36.9	2	1,513
ŀ	ogbg-molbbbp	24.1	26.0	2	2,039
ap.	NCI1	29.8	32.3	2	4,110
5	DD	284.3	715.7	2	1,178

## 40 A.2 Algorithms

We summarize the current GC algorithms in Table A2. We choose 12 representative ones for
evaluation in this paper including *Random*, *K-Center* [27], *Herding* [33], *GCond* [13], *DosCond* [12], *SGDD* [37], *GCDM* [18], *DM* [22], *SFGC* [42], *GEOM* [40], *KiDD* [36], *Mirage* [9]. We will
continue to update and improve the benchmark to include more algorithms. Here we introduce
the GC algorithms in detail:

#### **• Traditional Core-set Methods**

- 47 Random: For node classification tasks, nodes are randomly selected to form a new subgraph.
   48 For graph classification, the graphs are randomly selected to create a new subset.
- Herding [33]: The nodes or graphs are selected samples that are closest to the cluster center.
- **K-Center** [27]: Nodes or graphs are chosen such that they have the minimal distance to the nearest cluster center, which is generated using the K-Means Clustering method.

## 52 • Gradient Matching Methods

GCond [13]: In GCond, the optimization of the synthetic dataset is framed as a bi-level problem. It adapts a gradient matching scheme to match the gradients of GNN parameters between the condensed and original graphs, while optimizing the model's performance on the datasets. For generating the synthetic adjacency matrix, GCond employs a Multi-Layer Perceptron (MLP) to model the edges by using node features as input, maintaining the correlations between node features and graph structures.

<sup>59</sup> – **DosCond** [12]: In DosCond, the gradient matching scheme only matches the network <sup>60</sup> gradients for model initialization  $\theta_0$  while discarding the training trajectory of  $\theta_t$ , which <sup>61</sup> accelerated the entire condensation process by only informing the direction to update the

Table A2: Summary of Graph Condensation (GC) algorithms. We also provide public access to the official algorithm implementations. "KRR" is short for Kernel Ridge Regression and "CTC" is short for computation tree compression. "GNN" is short for Graph, "GNTK" is short for graph neural tangent kernel, "SD" is short for spectral decomposition. "NC" is short for node classification, "LP" is short for link prediction, "AD" is short for anomaly detection, and "GC" is short for graph classification.

Taxonomy	Method	Initialization	Backbone Model	Downstream Task	Code	Venue
Traditional	Random	_	_		_	_
Mathada	Herding [33]		_	_	link	ICML, 2009
Methods	K-Center [27]	_	_		link	ICLR, 2018
	GCond [13]	Random Sample	GNN	NC	link	ICLR, 2021
	DosCond [12]	Random Sample	GNN	NC, GC	link	SIGKDD, 2022
	MSGC [7]	Zero Matrix	GNN	NC	_	KBS, 2023
Gradient Matching	SGDD [37]	Random Sample	GNN	NC, LP, AD	link	NeurIPS, 2023
	GCARe [24]		GNN	NC	_	Appl. Sci. 2023
	CTRL [39]	K-Means	GNN	NC, GC	link	arxiv, 2024
	GroC [17]	Random Sample	GNN	NC, GC	_	arxiv, 2023
	EXGC <sup>[4]</sup>	Random Sample	GNN	NC	link <sup>1</sup>	WWW 2024
	MCond [8]	Random Sample	GNN	NC	_	ICDE, 2024
Distribution	GCDM [18]	Random Sample	GNN	NC	_	arxiv, 2022
Matching	DM [20, 22]	Random Sample	GNN	NC	_	ICDM, 2023
-	GDEM [19]	Eigenbasis Approximation	SD	NC	link	ICML, 2024
	FedGKD [26]	Random Noise	GNN	NC	_	arxiv, 2023
Trajectory	SFGC [42]	K-Center	GNN	NC	link	NeurIPS, 2023
Matching	GEOM [40]	K-Center	GNN	NC	link	ICML, 2024
VDD	GC-SNTK [31]	Random Noise	GNTK	NC	link	WWW, 2024
KKK	KiDD [36]	Random Sample	GNTK	GC	link	SIGKDD, 2023
CTC	Mirage [9]		GNN	GC	link	ICLR, 2024

<sup>1</sup> The code repository for EXGC is not fully developed.

synthetic dataset. DosCond also modeled the discrete graph structure as a probabilistic model and each element in the adjacency matrix follows a Bernoulli distribution.
<b>MSGC</b> [7]: MSGC condenses a large-scale graph into multiple small-scale sparse graphs, leveraging neighborhood patterns as substructures to enable the construction of various connection schemes. This process enriches the diversity of embeddings generated by GNNs, enhances the representation power of GNNs con complex graphs.
<b>SGDD</b> [37]: SGDD uses graphon approximation to ensure that the structural information of the original graph is retained in the synthetic, condensed graph. The condensed graph structure is optimized by minimizing the optimal transport (OT) distance between the original structure and the condensed structure.
<b>GCARe</b> [24]: GCARe addresses biases in condensed graphs by regularizing the condensation process, ensuring that the knowledge of different subgroups is distilled fairly into the resulting graphs.
<b>CTRL</b> [39]: CTRL clusters each class of the original graph into sub-clusters and uses these as initial value for the synthetic graph. By considering both the direction and magnitude of gradients during gradient matching, it effectively minimizes matching errors during the condensation phase.
<b>GroC</b> [17]: GroC uses an adversarial training (bi-level optimization) framework to explore the most impactful parameter spaces and employs a Shock Absorber operator to apply targeted adversarial perturbation.
<b>EXGC</b> [4]: EXGC leverages Mean-Field variational approximation to address inefficiency in the current gradient matching schemes and uses the Gradient Information Bottleneck objective to tackle node redundancy.
<b>MCond</b> [8]: MCond addresses the limitations of traditional condensed graphs in handling unseen data by learning a one-to-many node mapping from original nodes to synthetic nodes and uses an alternating optimization scheme to enhance the learning of synthetic graph and mapping matrix.

**•** Distribution Matching Methods

- GCDM [18]: GCDM synthesizes small graphs with receptive fields that share a similar distribution to the original graph, achieved through a distribution matching loss quantified by maximum mean discrepancy (MMD).
- DM [20, 22]: DM can be regarded as a one-step variant of GCDM. In DM, the optimization is centered on the initial parameters. Notably, in [20] and [22], DM does not learn any structures for efficiency. However, for better comparison in our experiments, we continue to learn the adjacency matrix.
- FedGKD [26]: FedGKD trains models on condensed local graphs within each client to mitigate the potential leakage of the training set membership. FedGKD features a Federated Graph Neural Network framework that enhances client collaboration using a task feature extractor for graph data distillation and a task relator for globally-aware model aggregation.

## **• Trajectory Matching Methods**

- SFGC [42]: SFGC uses trajectory matching instead of a gradient matching scheme. It first trains a set of GNNs on original graphs to acquire and store an expert parameter distribution offline. The expert trajectory guides the optimization of the condensed graph-free data. The generated graphs are evaluated using closed-form solutions of GNNs under the graph neural tangent kernel (GNTK) ridge regression, avoiding iterative GNN training.
- 107 GEOM [40]: GEOM makes the first attempt toward lossless graph condensation using 108 curriculum-based trajectory matching. A homophily-based difficulty score is assigned to 109 each node and the easy nodes are learned in the early stages while more difficult ones are 110 learned in the later stages. On top of that, GEOM incorporated a Knowledge Embedding 111 Extraction (KEE) loss into a matching loss.

#### • Kernel Ridge Regression Methods

- GC-SNTK [31]: GC-SNTK introduces a Structure-based Neural Tangent Kernel(SNTK)
   to capture graph topology, replacing the inner GNNs training in traditional GC paradigm,
   avoiding multiple iterations.
- KiDD [36]: KiDD uses kernel ridge regression (KRR) with a graph neural tangent kernel (GNTK) for graph-level tasks. To enhance efficiency, KiDD introduces LiteGNTK, a simplified GNTK, and proposes KiDD-LR for faster low-rank approximation and KiDD-D for handling discrete graph topology using the Gumbel-Max reparameterization trick. We use KiDD-LR for experiments as it has generally demonstrated better performance compared to KiDD-D.

#### **• Computation Tree Compression Methods**

 Mirage [9]: Mirage decomposes graphs in datasets into a collection of computation trees and then mines frequently co-occurring trees from this set. Mirage then uses aggregation functions (MEANPOOL, SUMPOOL, etc.) on the embeddings of the root node of each tree to approximate the graph embedding.

## 127 A.3 Hyper-Parameter Setting

For the implementation of various graph condensation methods, we adhere to the default parameters as specified by the authors in their respective original implementations. This approach ensures that our results are comparable to those reported in the foundational studies. For condensation ratios that were not explored in the original publications, we employ a grid search strategy to identify the optimal hyperparameters within the predefined search space. This includes experimenting with various combinations, such as differing learning rates for the feature optimizer and the adjacency matrix optimizer. The corresponding hyperparameter space are shown in Table A3.

#### 135 A.4 Computation resources

All experiments were conducted on a high-performance GPU cluster to ensure a fair comparison.
 The cluster consists of 32 identical dell-GPU nodes, each featuring 256GB of memory, 2 Intel Xeon
 processors, and 4 NVIDIA Tesla V100 GPUs, with each GPU having 64 GB of GPU memory. If any
 experiment setting exceeds the GPU memory limit, it is reported as out-of-memory (OOM).

Method	Hyperparameter	Values
General Settings	Learning Rate Epochs Layers Dropout Rate Weight Decay Hidden Units Pooling Activation Batch Size	0.1, 0.01, 0.001, 0.0001, 0.00001 300, 400, 500, 800, 1000, 2000, 3000, 4000, 5000 2, 3 0, 0.05, 0.1, 0.5, 0.6, 0.7, 0.8 0, 0.0005 128, 256 sum, mean LeakyReLU, ReLU, Sigmoid, Softmax (16,6000)
SGDD	mx_size opt_scale	50, 100 5, 10
GCond, DosCond, SGDD, GCDM, DM	outer loop	1, 2, 5, 10, 15, 20
GCond, SGDD, GCDM	inner loop	1, 5, 10, 15, 20
SFGC, GEOM	expert_epochs start_epoch teacher_epochs	50, 70, 100, 350, 600, 800, 1000, 1500, 1600, 1900 10, 20, 50, 100, 200, 300 800, 1000, 1200, 2400, 3000
GEOM	lam T scheduler	0.6, 0.7, 0.75, 0.8, 0.85, 0.9, 0.95 250, 500, 600, 800, 1000, 1200 linear, geom, root
KiDD	scale rank orth_reg	uniform, degree 8, 16, 32 0.01, 0.001, 0.0001

 Table A3: Hyperparameter search space of different methods

## 140 A.5 Discussion on Existing Benchmarks

To the best of our knowledge, the only concurrent work is GCondenser [21]. The comparison 141 of GCondser and our GC-Bench are list in Table A4. GCondenser [21] focus the node-level GC 142 methods for node classification on homogeneous graphs with limited evaluation dimensions in terms 143 of performance and time efficiency. Our GC-Bench analyzes more GC methods on a wider variety of 144 datasets (both homogeneous and heterogeneous) and tasks (node classification, graph classification), 145 146 encompassing both node-level and graph-level methods. In addition to performance and efficiency analysis, we further explore the transferability across different tasks (link prediction, node clustering, 147 anomaly detection) and backbones (GNN models and the popular Graph Transformer). With GC-148 Bench covering more in-depth investigation over a wider scope, we believe it will provide valuable 149 insights into existing works and future directions. 150

## **151 B Settings and Additional Results**

In this section, we provide more details of the experimental settings and the additional results for the proposed 6 research questions, respectively.

#### 154 B.1 Settings and Additional Results of Performance Comparison (RQ1)

#### 155 B.1.1 Comparison Setting

**Node Classification Graph Dataset Setting.** We compared ten state-of-the-art GC methods. The selection of the condensation ratio r is based on the labeling rates of different datasets. For datasets like *Cora* and *Citeseer*, the labeling rates are less than 50%, we select r as a proportion of the labeling rate, specifically at  $\{5\%, 10\%, 25\%, 50\%, 75\%, 100\%\}$ . For datasets like *ogbn-arxiv*, and inductive datasets where all nodes in the training graphs are labeled, with a relatively higher labeling rate, ris chosen to be  $\{5\%, 10\%, 25\%, 50\%, 75\%, 100\%\}$ . Corresponding condensation rates are shown in Table B2.

**Graph Classification Graph Dataset Setting.** We compared three state-of-the-art GC algorithms on graph classification datasets: *DosCond* [12], *KiDD* [36], and *Mirage* [9]. *Mirage* [9] does not condense datasets into unified graphs measurable by Graphs per Class(GPC) as *DosCond* [12] and

Ber	chmark Cov	verage	GCondenser	GC-Bench		
	Traditional	Core-set Methods	Random, K-Center	Random, K-Center, Herding		
thms	Gradient M	atching	GCond, DosCond, SGDD	GCond, DosCond, SGDD		
thr	Distribution	n Matching	GCDM. DM	GCDM, DM		
ori	Trajectory I	Matching	SFGC	SFGC. GEOM		
50 E	KRR	U	<u> </u>	KiDD		
A	CTC		_	Mirage		
	No de level	TT	Cora, Citeseer, ogbn-arxiv	Cora, Citeseer, ogbn-arxiv		
ets	Node-level	Homogenerous	Flickr, Reddit, PubMed	Flickr, Reddit		
tas	Node-level	Heterogenerous		ACM, DBLP		
)at	Graph laval			NCI1, DD, ogbg-molbace		
-	Graph-level	L	—	ogbg-molbbbp, ogbg-molhiv		
Tasks				node classification		
	Nodel-level		node classification	link prediction		
	Noucl-ievel		node classification	node clustering		
Ē				anomaly detection		
	Graph-level		—	graph classification		
	Condensation Ratios		$\checkmark$	$\checkmark$		
		Impact of Struture	structure v.s. structure-free	structure v.s. structure-free structure properties		
SUG	Perf	Struture		(Heterogeneity, Heterophily)		
ensic	1011.	Impact of Initialization	$\checkmark$	$\checkmark$		
uation Dim	Trans	Backbone Trans.	SGC and GCN transfer to SGC, GCN, GraphSAGE, APPNP, CHebyNet, MLP	SGC, GCN and Graph Transformer transfer to SGC, GCN, GraphSAGE, APPNP, ChebyNet, MLP, Graph Transformer		
Eval	Trans.	Task Trans.	_	node classification link prediction node clustering anomaly detection		
	Efficiency	Time	$\checkmark$	$\checkmark$		
	Enterency	Space	—	$\checkmark$		

Table A4: Comparison of GCondenser and GC-Bench

KiDD [36] do. Therefore, we measure the condensed dataset size by storing its elements in .pt format, 166 similar to DosCond [12] and KiDD [36]. We select the Mirage-condensed dataset size closest to 167 DosCond's as the corresponding GPC. KiDD [36] generally occupies more disk space than DosCond 168 under the same GPC. The size of *Mirage* datasets is determined by two parameters: the number of 169 GNN layers (L) and the frequency threshold  $\Theta$ . We fix L = 2, consistent with the 2-layer model used 170 for validation, and employ a grid search strategy to identify the threshold combination that yields a 171 dataset size closest to the targeted GPC. The corresponding disk space, GPC, and threshold choices 172 are presented in Table B1. Note that for small thresholds, the MP Tree search algorithms used in 173 Mirage [9] may reach recursive limits. Consequently, in DD and ogbg-molbace, certain GPCs lack 174 corresponding threshold values. 175

Heterogeneous Graph Dataset Setting. Due to the absence of condensation methods specifically
for heterogeneous graphs, we convert heterogeneous datasets into homogeneous graphs for condensation, focusing on target nodes. We uniformly summed the adjacency matrices corresponding to
various meta-paths as in [23], and applied zero-padding to match the maximum feature dimension as
well as one-hot encoding for nodes without features. Specifically, in *GEOM* [40], when calculating
heterophily, all nodes without labels (non-target nodes) are assigned the same distinct label, ensuring
a consistent heterophily calculation.

## 183 B.1.2 Additional Results

The graph classification performance on GCN is shown in Table B3. *DosCond* [12] with GCN demonstrates significant advantages in 12 out of 25 cases, while *KiDD* [36] underperforms in most scenarios. Notably, *DosCond* [12] and *Mirage* [9] even outperform the results of the whole dataset on

Dataset	Graph/ Cls	Mirage Disk Size (Bytes)	DosCond Disk Size (Bytes)	Class 0 Threshold	Class 1 Threshold
NCII [29]	$     \begin{array}{c}       1 \\       5 \\       10 \\       20 \\       50     \end{array} $	14,455 81,622 142,228 195,609 995,277	18,425 82,745 162,301 324,035 806,403	451 351 301 251 201	441 381 291 231 171
DD [3]	$     \begin{array}{c}       1 \\       5 \\       10 \\       20 \\       50     \end{array} $	38,352	855,077 4,265,957 8,529,583 17,056,751 42,638,383	15 	9
ogbg-molbace [11]	$     \begin{array}{c}       1 \\       5 \\       10 \\       20 \\       50     \end{array} $	13,836 60,047 106,077 232,191	14143 60,927 119,497 236,489 587,337	120 230 120 140	90 80 80 70
ogbg-molbbbp [11]	$     \begin{array}{c}       1 \\       5 \\       10 \\       20 \\       50     \end{array} $	8,817 34,699 66,433 104,091 324,425	8,831 34,175 65,929 129,289 319,369	29 49 30 20 17	198 109 90 80 87
ogbg-molhiv [11]	$     \begin{array}{c}       1 \\       5 \\       10 \\       20 \\       50     \end{array} $	9,606 54,669 74,524 148,028 330,498	9,717 38,837 75,263 148,095 366,463	8,000 1,760 1,680 1,420 800	250 170 130 110 110

Table B1: Comparison of Disk Size and Graph per Class (GPC) for condensed datasets between *Mirage* and *DosCond*.

Table B2: Different condensation ratios of transductive datasets. For heterogeneous datasets, the number of nodes in the original graph is the sum of all types of nodes.

Ratio (r)	Cora	Citeseer	ACM	DBLP
5%	0.26%	0.18%	0.003%	0.002%
10%	0.52%	0.36%	0.007%	0.004%
25%	1.30%	0.90%	0.013%	0.007%
50%	2.60%	1.80%	0.033%	0.019%
75%	3.90%	2.70%	0.066%	0.037%
100%	5.20%	3.60%	0.332%	0.186%

*ogbg-molbace*. For *Mirage* [9], due to the algorithm's recursive depth under low threshold parameters,
we have only one result corresponding to GPC 1 on *DD*. However, this single result already surpasses

all datasets condensed by *KiDD* [36] and the dataset with GPC 1 condensed by *DosCond*.

#### 190 B.2 Settings and Additional Results of Structure in Graph Condensation (RQ2)

#### 191 B.2.1 Experimental Settings

The homophily ratio we use is the edge homophily ratio, which represents the fraction of edges that connect nodes with the same labels. It can be calculated as:

$$\mathcal{H}(G) = \frac{1}{|\mathcal{E}|} \sum_{(j,k)\in\mathcal{E}} \mathbf{1}(y_j = y_k), \ i \in \mathcal{V},$$
(A.1)

where  $\mathcal{V}$  is the node set,  $\mathcal{E}$  is the edge set,  $|\mathcal{E}|$  is the number of edges in the graph,  $y_i$  is the label of node *i* and  $\mathbf{1}(\cdot)$  is the indicator function. A graph is typically considered to be highly homophilous when  $\mathcal{H}$  is large (typically,  $0.5 \leq \mathcal{H} \leq 1$ ), such as *Cora* and *Reddit*. Conversely, a graph with a low edge homophily ratio is considered to be heterophilous, such as *Flickr*.

We also calculate the homophily ratio of condensed datasets. Since the condensed datasets have weighted edges, we first sparsify the graph by removing all edges with weights less than 0.05,

Dataset	Graph	Ratio(r)	Traditio	nal Core-set	methods	Gradient	KRR	СТС	Whole
Duniser	/Cls	111110(/)	Random	Herding	K-Center	DosCond	KiDD	Mirage	Dataset
	1	0.06%	$53.30_{\pm 0.6}$	$55.20_{\pm 2.6}$	$55.20 \pm 2.6$	57.30±0.9	$49.30_{\pm 1.1}$	$49.10_{\pm 0.9}$	
NCH	5	0.24%	$55.00_{\pm 1.4}$	$56.50 \pm 0.9$	$53.20_{\pm 0.6}$	<b>58.40</b> ±1.4	$56.10_{\pm 1.0}$	$49.60_{\pm 2.2}$	
$\Lambda_{CC}$ (%)	10	0.49%	$58.10_{\pm 2.2}$	$58.60_{\pm 0.8}$	$57.00_{\pm 2.6}$	$57.80_{\pm 1.6}$	$57.50_{\pm 1.1}$	$48.60_{\pm 0.1}$	$71.1_{\pm 0.8}$
<i>I</i> .( <i>n</i> )	20	0.97%	$54.40_{\pm 0.8}$	$59.10_{\pm 1.1}$	<b>60.10</b> ±1.3	$60.10_{\pm 3.2}$	$56.40_{\pm 0.6}$	$48.70_{\pm 0.0}$	
	50	2.43%	$56.80_{\pm 1.1}$	$58.70_{\pm 1.1}$	$64.40_{\pm 0.9}$	$58.20_{\pm 2.8}$	$59.90_{\pm 0.6}$	$48.60_{\pm 0.1}$	
	1	0.21%	$59.70_{\pm 1.5}$	$66.90_{\pm 2.8}$	$66.90_{\pm 2.8}$	$68.30_{\pm 6.6}$	$58.60_{\pm 2.4}$	$71.20_{\pm 6.6}$	
ממ	5	1.06%	$61.90_{\pm 1.1}$	$66.20_{\pm 2.5}$	$62.00_{\pm 1.7}$	$73.10_{\pm 2.2}$	$58.60_{\pm 1.1}$	-	
$\Delta cc_{\rm c}$ (%)	10	2.12%	$63.70_{\pm 2.8}$	$68.00_{\pm 3.6}$	$62.50_{\pm 2.3}$	$71.30_{\pm 8.3}$	$61.60_{\pm 3.8}$	-	$78.4_{\pm 1.7}$
Acc. (70)	20	4.25%	$64.70_{\pm 5.3}$	$69.70_{\pm 0.8}$	$63.10_{\pm 1.9}$	$73.00_{\pm 5.8}$	$62.60_{\pm 1.4}$	-	
	50	10.62%	$66.60_{\pm 2.1}$	$68.50_{\pm 1.4}$	$68.90 \pm 1.8$	<b>74.20</b> ±3.6	$59.30_{\pm 0.0}$	-	
	1	0.17%	$0.510_{\pm .083}$	$0.515_{\pm .040}$	$0.517_{\pm.044}$	$0.658 \pm 0.000$	$0.568_{\pm.047}$	$0.733_{\pm.012}$	
oaha molhaca	5	0.83%	$0.612_{\pm.036}$	$0.653_{\pm .043}$	$0.508_{\pm.087}$	$0.691_{\pm.06}$	$0.356_{\pm.022}$	$0.760_{\pm.002}$	
ROC-AUC	10	1.65%	$0.620_{\pm .054}$	$0.658_{\pm.046}$	$0.646_{\pm.047}$	$0.702_{\pm.045}$	$0.542_{\pm.027}$	$0.759_{\pm.002}$	$0.711_{\pm.019}$
Roc-noc	20	3.31%	$0.642_{\pm.053}$	$0.631_{\pm.051}$	$0.575_{\pm.03}$	$0.659_{\pm.049}$	$0.526_{\pm.014}$	$0.761_{\pm.003}$	
	50	8.26%	$0.677_{\pm.015}$	$0.629_{\pm .053}$	$0.576_{\pm .087}$	$0.714_{\pm.032}$	$0.446_{\pm .042}$	-	
	1	0.12%	$0.534_{\pm.041}$	$0.560_{\pm.017}$	$0.560_{\pm.017}$	$0.600_{\pm .023}$	$0.504_{\pm .042}$	$0.600_{\pm .002}$	
ogha molhhhn	5	0.61%	$0.561_{\pm.014}$	$0.574_{\pm.022}$	$0.585_{\pm.005}$	$0.579_{\pm.056}$	$0.561_{\pm.004}$	$0.609_{\pm.061}$	
ROC-AUC	10	1.23%	$0.566_{\pm.011}$	$0.590_{\pm .024}$	$0.598_{\pm.025}$	$0.556_{\pm.063}$	$0.550_{\pm .005}$	$0.517_{\pm .028}$	$0.646_{\pm.013}$
Roc-noc	20	2.45%	$0.593_{\pm.023}$	$0.568 \pm .019$	$0.545_{\pm.009}$	$0.590_{\pm .057}$	$0.594_{\pm.022}$	$0.626_{\pm.032}$	
	50	6.13%	$0.587_{\pm.007}$	$0.579_{\pm.022}$	$0.621_{\pm.011}$	$0.598_{\pm.024}$	$0.603_{\pm.01}$	$0.602_{\pm.018}$	
	1	0.01%	$0.733_{\pm.008}$	$0.727_{\pm.012}$	$0.727_{\pm.012}$	$0.734_{\pm.002}$	$0.725_{\pm.007}$	$0.728_{\pm.012}$	
oghg-molhiv	5	0.03%	$0.729_{\pm.006}$	$0.720_{\pm .018}$	$0.739_{\pm.01}$	$0.736_{\pm.008}$	$0.738 \pm 0.003$	$0.717_{\pm.003}$	
ROC-AUC	10	0.06%	$0.724_{\pm.011}$	$0.726_{\pm.014}$	$0.723_{\pm.012}$	$0.736_{\pm.007}$	$0.731_{\pm.008}$	$0.735_{\pm.028}$	$0.750_{\pm.010}$
NOC-AUC	20	0.12%	$0.723_{\pm.015}$	$0.726_{\pm.015}$	$0.724_{\pm.01}$	$0.733_{\pm.007}$	$0.703_{\pm .097}$	$0.710_{\pm .016}$	
	50	0.30%	$0.712_{\pm.014}$	$0.723_{\pm.019}$	$0.721_{\pm.012}$	$0.731_{\pm.011}$	$0.723_{\pm.011}$	$0.718_{\pm.022}$	

Table B3: **Graph classification performance on GCN** (mean $\pm$ std) across datasets with varying condensation ratios *r*. The best results are shown in **bold** and the runner-ups are shown in **underlined**. Red color highlights entries that exceed the whole dataset values.

\**Mirage* cannot directly generate graphs with the required ratio. Thus, we search the parameter space and aligned the generated graph to match *DosCond*'s disk usage as substitution (see Appendix B.1).

then calculate the homophily ratio by adjusting the fraction to a weighted fraction, which can be represented as:

$$\mathcal{H}(G) = \frac{\sum_{(j,k)\in\mathcal{E}} w_{jk} \mathbf{1}(y_j = y_k)}{\sum_{(j,k)\in\mathcal{E}} w_{jk}}, \ i \in \mathcal{V},$$
(A.2)

where  $w_{jk}$  is the weight of the edge between nodes j and k.

## 203 B.2.2 Additional Results

The results of homophily ratios of condensed datasets are shown in Table B4. It appears that condensed datasets often struggle to preserve the homophily properties of the original datasets. For instance, in the case of the heterophilous dataset *Flickr*, an increase in the homophily rate is observed under most methods and ratios.

	Whole Dataset	Ratio $(r)$	GCDM	DM	DosCond	GCond	SGDD
Cora	0.81	1.30% 2.60% 5.20%	0.76 0.11 1.00	0.88 0.74 0.21	0.20 0.16 0.15	0.64 0.55 0.62	0.19 0.19 0.15
Citeseer	0.74	0.90% 1.80% 3.60%	0.16 0.08 1.00	0.75 0.30 0.34	0.19 0.20 0.15	0.57 0.36 0.22	0.14 0.19 0.15
Flickr	0.24	$0.05\% \\ 0.50\% \\ 1.00\%$	0.28 0.29 0.36	0.29 ↑ 0.22↓ 0.18 ↓	0.25 0.08 0.06	0.28 0.28 0.28	0.32 0.30 0.26

Table B4: Homophily ratio comparison of different condensed datasets

We visualize the condensed datasets using force-directed graph visualization, as shown in Figure B.1, Figure B.2, and Figure B.3. Since SFGC [42] and GEOM [40] synthesize edge-free datasets, we do not visualize the datasets they condensed. As shown in the visualization, graphs condensed
 by different methods exhibit distinct structural characteristics. For example, distribution matching
 methods often result in less pronounced community structures compared to other methods.

We also visualize the node degree distribution of the original graph and the condesed graphs in Figure B.4. Note that the graphs condensed by *GCDM* [18] and *DM* [22] are dense and each edge has an extremely small weight under most situations, the degree of each node is also small. We observe that the degree distributions of most condensed datasets deviate significantly from the original graph. Among them, *SGDD* [37] demonstrates a relatively similar degree distribution to that of the original graph.



Figure B.1: Visualization of the Condensed *Citeseer* (1.80%) Dataset. Only the top 20% of edges ranked by weight are visualized.



Figure B.2: Visualization of the Condensed *Cora* (2.60%) Dataset. Only the top 20% of edges ranked by weight are visualized.



Figure B.3: Visualization of the Condensed *Flickr* (0.50%) Dataset. Only the top 1% of edges ranked by weight are visualized.

#### 219 B.3 Settings and Additional Results of Transferability in Different Tasks (RQ3)

#### 220 B.3.1 Link Prediction

For the link prediction task, we utilize a graph autoencoder (GAE)[15] based on Graph Convolutional Networks (GCN[14]). The GAE consists of a two-layer GCN encoder that creates node embeddings. During training, we enhance the dataset by randomly adding negative links and use a decoder to perform binary classification on edges. During evaluation, we test the model using the test set of the original graph. Since trajectory matching methods do not generate any edges, we do not use them for link prediction tasks. The results of condensed datasets on the link prediction task are shown in



Figure B.4: Degree distribution in the condensed graphs for *Citeseer* (1.80%), *Cora* (2.60%), and *Flickr* (0.05%). The first, second, and third columns correspond to *Citeseer*, *Cora*, and *Flickr*, respectively.

Table B5. We observe that most condensed datasets underperform in link prediction tasks, especially on *ogbn-arxiv* and *Flickr*. Most methods' condensed datasets consistently underperform compared to traditional core-set methods, indicating room for improvement.

## 230 B.3.2 Node Clustering

For the node clustering tasks on condensed datasets, we utilize DAEGC [30] to train on synthetic datasets condensed using the node classification task. We then test the trained model on the original large-scale datasets and include the results of other methods on the original graph for comprehensive comparison. Due to the performance degradation of GAT with large neighborhood sizes, we use GCN as the encoder.Performance metrics include Accuracy (Acc.), Normalized Mutual Information (NMI), F-score, and Adjusted Rand Index (ARI).

To fully leverage the condensed datasets, we include the results of node clustering with pertaining. In this experiment, the GCN encoder is first trained on the synthetic datasets with a node classification task, which incorporates the synthetic labels' information. Using the pre-trained GCN as an encoder, we then perform node clustering on the synthetic datasets and the original graph. Results of node clustering tasks, both without and with pertaining are shown in Table B6 and Table B7 respectively. We observe that most condensed datasets perform worse in the node clustering task compared to the original dataset. However, when additional information from the pretraining of the node classification

Dataset	Ratio (r)	Random	Herding	K-Center	GCDM	DM	DosCond	GCond	SGDD	Whole Dataset
	0.90%	0.52	0.52	0.55	0.53	0.53	0.50	0.65	0.69	
Citeseer	1.80%	0.52	0.52	0.54	0.51	0.52	0.51	0.51	0.67	0.82
	3.60%	0.54	0.53	0.53	0.53	0.53	0.53	0.53	0.61	
	1.30%	0.58	0.54	0.58	0.72	0.71	0.67	0.61	0.51	
Cora	2.60%	0.55	0.55	0.56	0.69	0.67	0.58	0.77	0.62	0.78
	5.20%	0.57	0.56	0.58	0.70	0.71	0.59	0.65	0.56	
	0.05%	0.76	0.68	0.67	0.66	0.68	0.63	0.60	0.70	
ogbn-arxiv	0.20%	0.72	0.72	0.73	0.72	0.72	0.69	0.71	0.51	0.75
0	0.50%	0.74	0.73	0.74	0.71	0.73	0.72	0.72	0.70	
	0.05%	0.55	0.54	0.53	0.60	0.53	0.52	0.54	0.51	
Flickr	0.20%	0.63	0.63	0.63	0.63	0.51	0.53	0.57	0.70	0.75
	0.50%	0.70	0.68	0.70	0.56	0.65	0.62	0.67	0.61	

Table B5: Link Prediction Accuracy (%) of different condensed datasets. The best results are shown in **bold**.

task on condensed dataset is utilized, the results of node clustering significantly improve. Notably, some datasets in Table B6 exhibit identical results with the Adjusted Rand Index (ARI) being 0 or even negative. This occurs because the clustering results do not match the number of classes in the labels, requiring manual splitting of clusters in such scenarios. An ARI of 0 indicates that the clustering result is as good as random, while a negative ARI suggests it is worse than random.

## 249 **B.3.3** Anomaly Detection

For the anomaly detection tasks, we generate two types of anomalies, *Contextual Anomalies* and *Structural Anomalies*, following the method described in [2]. We set the anomaly rate to 0.05; if the condensed dataset is too small, we inject one contextual anomaly and two structural anomalies.

**Contextual Anomalies**: Each outlier is generated by randomly selecting a node and substituting its attributes with those from another node with the maximum Euclidean distance in attribute space.

Structural Anomalies: Outliers are generated by randomly selecting a small group of nodes and
 making them fully connected, forming a clique. The nodes in this clique are then regarded as structural
 outliers. This process is repeated iteratively until a predefined number of cliques are generated.

We conduct anomaly detection by training a DOMINANT model [2], which features a shared graph 258 convolutional encoder, a structure reconstruction decoder, and an attribute reconstruction decoder. 259 Initially, we inject predefined anomalies into the test set of the original graph and use it for evaluation 260 across different condensed datasets derived from this graph. The model is then trained on these 261 condensed datasets, which were injected with specific types of anomalies before training. The 262 DOMINANT model measures reconstruction errors as anomaly scores for both the graph structure 263 and node attributes, combining these scores to detect anomalies. The results are evaluated using the 264 ROC-AUC metric, as shown in Table B8 and B9. 265

# B.4 Settings and Additional Results of Transferability across Backbone Model Architectures (RQ4)

## 268 B.4.1 Experimental Settings

For transferability evaluation, we use different models as backbones to test the condensation methods. For distribution matching methods, two backbone models with shared parameters are used to generate embeddings that are matched. For trajectory matching methods, two backbone models are used to generate expert trajectories and student trajectories, respectively, to match the corresponding parameters. For gradient matching methods, two backbone models with shared parameters are used to generate gradients for real and synthetic data. Models are selected using grid-searched hyperparameters. The details of the backbone architecture are as follows:

• MLP: MLP is a simple neural network consisting of fully connected layers. The MLP we use is structured similarly to a GCN but without the adjacency matrix input, effectively functioning

			Cite	seer				Сог	ra	
Methods	Ratio (r)	Acc.	NMI	ARI	F1	Ratio(r)	Acc.	NMI	ARI	F1
K-means		54.4	31.2	28.5	41.3		50.0	31.7	37.6	23.9
DAEGC [30]	Full	67.2	39.7	41.0	63.6	Full	70.4	52.8	68.2	49.6
	0.90%	40.6	19.1	17.5	36.0	1.30%	36.6	13.5	9.0	34.3
Random	1.80% 3.60%	$38.3 \\ 41.8$	$\begin{array}{c} 14.8\\ 18.1 \end{array}$	13.6 16.9	34.5 39.4	2.60% 5.20%	33.5 30.2	13.9 0.4	$\begin{array}{c} 7.1 \\ 0.0 \end{array}$	33.4 6.8
TT 1'	0.90%	41.9	16.9	15.3	40.0	1.30%	37.4	18.2	11.7	35.0
Herding	3.60%	44.9 58.1	27.8	29.2	41.1 52.3	2.00% 5.20%	36.6 26.7	13.7	2.9	34.0 20.6
W.C.	0.90%	37.9	13.4	11.1	35.2	1.30%	34.3	13.5	7.8	32.4
K-Center	1.80% 3.60%	30.0 31.9	25.5 14.0	10.2	40.5 31.0	5.20%	42.5 30.2	0.4	0.0	42.5 6.8
	0.90%	41.4	16.9	16.2	38.6	1.30%	30.2	0.4	0.0	6.8
GCDM	3.60%	22.8	18.1	18.1	38.8 20.9	5.20%	30.2 30.2	0.4	0.0	6.8
	0.90%	23.5	2.1	1.1	17.7	1.30%	30.2	0.4	0.0	6.8
DM	3.60%	43.5 25.9	4.5	3.5	42.9 20.0	2.00% 5.20%	29.2 30.2	2.0 0.4	0.0	9.3 6.8
	0.90%	28.6	10.2	6.3	25.1	1.30%	30.2	0.4	0.0	6.8
DosCond	3.60%	44.3	20.6	17.0	49.5 38.6	5.20%	29.6	16.2	7.7	23.4
	0.90%	$\frac{61.8}{50.6}$	$\frac{34.0}{22.0}$	$\frac{34.7}{22.6}$	55.9	1.30%	46.6	36.7	27.3	41.2
GCond	3.60%	57.8	32.0	30.2	50.5 54.8	5.20%	49.9	40.9	27.9	37.3
CODD	0.90%	56.5	27.3	26.8	50.6	1.30%	30.2	0.4	0.0	6.8
SGDD	3.60%	42.5	24.0	20.0	38.2	5.20%	33.2	17.9	8.8	25.5
	0.90%	46.7	19.9	18.8	43.4	1.30%	42.1	23.5	17.7	39.2
SFGC	3.60%	47.7	27.4 19.0	27.0 16.9	52.8 45.3	5.20%	$\frac{34.4}{30.1}$	0.4	-0.1	6.8
	0.90%	41.4	16.9	16.2	38.6	1.30%	40.7	16.9	11.6	37.3
GEOM	1.80% 3.60%	44.1 22.8	18.1	18.1	38.8 20.9	5.20%	30.8 35.6	12.9	9.3 11.5	29.2 33.6

Table B6: Node Clustering without Pretraining Results on *Cora* and *Citeseer* with varying condensation ratios (r). The best results are highlighted in **bold**, the runner-ups are <u>underlined</u>, and the best results of condensed datasets are shaded in gray.

as a standard multi-layer perceptron (MLP). The MLP we adopted consists of 2 layers with 256
 hidden units in each layer.

• GCN [14]: GCN is the most common architecture for evaluating condensed datasets in main-280 stream GC methods. GCN defines a localized, first-order approximation of spectral graph 281 convolutions, effectively aggregating and combining features from a node's local neighborhood, 282 leveraging the graph's adjacency matrix to update node representations through multiple layers. 283 We adhere to the setting in previous work [13] and use 2 graph convolutional layers for node 284 classification, each followed by ReLu activation and batch normalization depending on the config-285 286 uration. For graph classification, we use a 3-layer GCN with a sum pooling function. The hidden unit size is set to 256. 287

SGC [34]: SGC is the standardized model used for condensation in previous works. It can be regarded as a simplified version of GCN, which ignores the nonlinear activation function but still keeps two Graph Convolution layers, thereby preserving similar graph filtering behaviors. In the experiments, we use 2-layer SGC with no bias.

• **Cheby** [1]: Cheby utilizes Chebyshev polynomials to approximate the graph convolution operations, which retains the essential graph filtering properties of GCN while reducing the com-

			Cite	seer			Cora				
Methods	Ratio $(r)$	Acc.	NMI	ARI	<b>F1</b>	Ratio $(r)$	Acc.	NMI	ARI	F1	
Random	0.90% 1.80% 3.60%	27.3 32.7 44.6	5.5 9.7 16.0	4.7 7.8 14.1	24.6 31.4 43.0	1.30% 2.60% 5.20%	41.7 36.5 44.4	15.8 14.6 23.5	13.5 9.1 14.9	37.3 35.4 45.7	
Herding	$0.90\% \\ 1.80\% \\ 3.60\%$	36.7 36.8 39.4	12.8 13.1 16.9	11.1 10.2 14.1	34.4 36.2 38.1	1.30% 2.60% 5.20%	40.7 36.1 35.0	18.3 14.6 16.6	12.9 8.7 10.9	40.0 34.9 32.0	
K-Center	0.90% 1.80% 3.60%	33.7 37.6 41.7	9.7 15.6 17.1	8.3 13.9 14.3	29.5 34.9 40.5	1.30% 2.60% 5.20%	41.8 38.5 38.5	19.3 20.8 17.4	14.5 14.8 10.9	39.2 38.3 36.3	
GCDM	0.90% 1.80% 3.60%	31.1 33.1 39.7	9.6 11.9 18.0	6.6 11.1 15.2	27.3 30.4 34.4	1.30% 2.60% 5.20%	21.3 27.0 30.0	3.7 10.9 12.4	1.7 5.7 7.0	20.1 26.7 29.6	
DM	$0.90\% \\ 1.80\% \\ 3.60\%$	36.5 37.1 29.2	15.7 10.6 6.0	12.9 8.6 4.0	30.0 31.4 23.6	1.30% 2.60% 5.20%	27.3 20.8 23.5	9.3 3.3 4.8	4.5 0.9 1.6	25.7 19.0 16.3	
DosCond	$0.90\% \\ 1.80\% \\ 3.60\%$	<b>62.7</b> 45.2 58.6	<b>35.9</b> 17.9 29.6	<b>35.1</b> 15.4 28.5	<b>60.6</b> 40.8 55.8	1.30% 2.60% 5.20%	60.2 44.5 25.4	42.5 30.1 9.8	29.4 16.6 5.0	61.2 46.5 25.0	
GCond	0.90% 1.80% 3.60%	44.0 58.5 52.0	22.5 30.9 26.8	$     \begin{array}{r}       18.7 \\       29.6 \\       22.5     \end{array} $	40.3 54.9 46.6	1.30% 2.60% 5.20%		45.1 44.5 47.1	$     \frac{40.4}{36.2}     37.1 $		
SGDD	$0.90\% \\ 1.80\% \\ 3.60\%$	46.7 55.4 40.5	23.5 28.0 18.3	19.1 25.8 14.3	42.3 50.9 34.8	1.30% 2.60% 5.20%	65.1 35.7 <b>74.8</b>	44.6 19.2 <b>51.9</b>	37.1 11.7 <b>53.1</b>	64.6 34.8 <b>72.8</b>	
SFGC	0.90% 1.80% 3.60%	34.2 47.1 48.5	9.8 21.7 23.3	8.4 20.6 21.5	32.2 43.5 44.8	1.30% 2.60% 5.20%	41.2 38.7 37.3	21.2 20.7 21.1	13.9 13.5 14.4	40.2 36.2 34.1	
GEOM	0.90% 1.80% 3.60%	32.7 48.2 54.2	10.5 23.6 25.7	8.6 22.7 24.9	31.7 45.2 52.1	1.30% 2.60% 5.20%	39.1 32.2 38.1	20.1 14.5 22.0	11.4 8.9 12.7	40.0 29.4 34.7	

Table B7: **Node Clustering with Pretraining Results** on *Cora* and *Citeseer* with varying condensation ratios (*r*). The best results are highlighted in **bold** and the runner-ups are underlined.

Table B8: **Structural Anomaly Detection results (ROC-AUC)** on *Cora* and *Citeseer* with varying condensation ratios. The best results are shown in **bold** and the runner-ups are shown in <u>underline</u>.

Dataset	Ratio (r)	Random	Herding	K-Center	GCDM	DM	DosCond	GCond	SGDD	SFGC	GEOM
Citeseer	0.90%	0.44	0.38	0.44	0.76	0.76	0.73	<b>0.77</b>	0.67	0.62	0.59
	1.80%	0.46	0.45	0.46	0.78	0.78	0.66	<u>0.75</u>	0.68	0.60	0.56
	3.60%	0.44	0.40	0.44	0.76	0.76	0.70	<u>0.74</u>	<u>0.75</u>	0.59	0.57
Cora	1.30%	0.56	0.59	0.62	0.80	0.80	0.79	<b>0.81</b>	0.75	0.54	0.51
	2.60%	0.50	0.65	0.67	0.80	0.80	<b>0.82</b>	0.79	0.81	0.53	0.53
	5.20%	0.65	0.55	0.67	<b>0.82</b>	0.82	<b>0.82</b>	<u>0.81</u>	0.71	0.54	0.55

putational complexity. We use a 2-layer Cheby with 256 hidden units and ReLU activation
 function.

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• **GraphSAGE** [10]: GraphSAGE is a spatial-based graph neural network that directly samples and aggregates features from a node's local neighborhood. In the experiments, We use a two-layer architecture and a hidden dimension size of 256 while using a mean aggregator.

• **APPNP [16]:** APPNP leverages personalized PageRank to propagate information throughout the graph. This method decouples the neural network used for prediction from the propagation mechanism, enabling the use of personalized PageRank for message passing. In the experiments, we use a 2-layer model implemented with ReLU activation and sparse dropout to condense and evaluate.

Dataset	Ratio (r)	Random	Herding	K-Center	GCDM	DM	DosCond	GCond	SGDD	SFGC	GEOM
	0.90%	0.62	0.60	0.62	0.65	0.65	0.55	0.70	0.74	0.62	0.59
Citeseer	1.80%	0.60	0.54	0.60	0.64	0.65	0.58	0.68	0.67	0.60	0.56
	3.60%	0.57	0.56	0.57	0.68	0.68	0.59	0.68	0.52	0.59	0.57
	1.30%	0.52	0.48	0.53	0.52	0.52	0.45	0.54	0.41	0.54	0.51
Cora	2.60%	0.50	0.45	0.54	0.54	0.54	0.56	0.55	0.57	0.53	0.53
	5.20%	0.56	0.58	0.59	0.55	0.55	0.55	0.57	0.62	0.54	0.55

Table B9: **Contextual Anomaly Detection results (ROC-AUC)** on *Cora* and *Citeseer* with varying condensation ratios. The best results are shown in **bold** and the runner-ups are shown in <u>underline</u>.

GIN [35]: GIN aggregates features by linearly combining the node features with those of their neighbors, achieving classification power as strong as the Weisfeiler-Lehman graph isomorphism test. We specifically applied a 3-layer GIN with a mean pooling function to compress and evaluate graph classification datasets. For the datasets *DD* and *NCI1*, we use negative log-likelihood loss function for training and softmax activation in the final layer. For *ogbg-molbace*, we use binary cross-entropy with logits and sigmoid activation in the final layer.

 Graph Transformer [28]: The Graph Transformer leverages the self-attention mechanism of the Transformer to capture long-range dependencies between nodes in a graph. It employs multi-head self-attention to dynamically weigh the importance of different nodes, effectively modeling complex relationships within the graph. We use a two-layer model with layer normalization and gated residual connections, following the settings outlined in [28].

### 316 **B.4.2** Additional Results

Table B10 shows the node classification accuracy of datasets condensed by traditional core-set methods, which is backbone-free, evaluated across different backbone architectures on *Cora*.

Table B10: **Node Classification Accuracy** (%) of core-set datasets across different backbone architectures on *Cora* (2.6%).

Methods	SGC	GCN	GraphSage	APPNP	Cheby	GTrans.	MLP
Full Dataset	80.8	80.8	80.8	80.3	78.8	69.6	81.0
Herding	74.8	74.0	74.1	73.3	69.6	65.4	74.1
K-Center	72.5	72.4	71.8	71.5	63.0	64.3	72.2
Random	71.7	72.4	71.6	71.3	65.3	62.7	71.6

#### 319 B.5 Settings and Additional Results of Initialization Impacts (RQ5)

## 320 B.5.1 Experimental Settings

- 321 The details of evaluated initialization mechanism are as follows:
- **Random Sample.** We randomly select features from nodes in the original graph that correspond to the same label, using these features to initialize the synthetic nodes.
- **Random Noise.** Consistent with prevalent dataset condensation methods, we initialize node features by sampling from a Gaussian distribution.

• **Center.** This method involves extracting features from nodes within the same label, applying the K-Means clustering algorithm to these features while treating the graph as a singular cluster and utilizing the centroid of this cluster as the initialization point for all synthetic nodes bearing the same label.

• **K-Center.** Similar to the Center initialization method, but employ the K-Means Clustering method on original nodes by dividing each class of the original graph nodes into n clusters, where n is the number of synthetic nodes per class. We select the center of these clusters as the initialization of synthetic nodes in this class. • **K-Means.** Similar to the K-Center initialization method, but instead of using the centroids of clusters to initialize the synthetic dataset, randomly select one node from each cluster to serve as the initial state for the synthetic node.

#### 337 B.5.2 Additional Results

The performance of different initialization mechanism on Cora (2.6%) and Cora (0.26%) are shown

in Table B11 and Table B12, respectively. It is evident that distribution matching methods are highly

sensitive to the choice of initialization, especially when the dataset is condensed to a smaller scale.
 Additionally, trajectory matching methods perform poorly with random noise initialization and often

fail to converge.

Table B11: Performance comparison of differ-<br/>ent initialization on various methods for *Cora* ent initialization on various methods for *Cora*<br/>(2.60%). The best results are shown in **bold**.Cora<br/>(0.26%). The best results are shown in **bold**.

Methods	Random Noise	Random Sample	Center	K-Center	K-Means	Methods	Random Noise	Random Sample	Center	K-Center	K-Means
GCDM	34.5	73.3	77.4	78.7	75.9	GCDM	32.3	37.8	78.7	78.7	34.3
DM	34.5	73.7	77.7	78.1	75.9	DM	32.2	38.4	77.9	77.9	34.2
DosCond	78.8	81.9	81.8	82.5	81.8	DosCond	78.7	82.4	80.5	82.0	81.9
GCond	74.8	75.1	76.3	76.2	75.1	GCond	80.2	81.6	80.1	81.2	80.7
SGDD	81.7	81.8	82.6	82.7	82.5	SGDD	82.2	82.2	82.7	82.7	81.5
SFGC	52.5	80.7	79.7	81.5	81.8	SFGC	79.7	79.7	79.8	79.8	72.0
GEOM	-	77.9	48.3	78.8	78.9	GEOM	-	49.6	51.3	51.3	65.0

342

#### 343 B.6 Settings and Additional Results of Efficiency and Scalability (RQ6)

#### 344 **B.6.1 Experimental Settings**

For a fair comparison, all the experiments are conducted on a single NVIDIA A100 GPU. Then we report the overall condensation time (min) when achieving the best validation performance, the peak CPU memory usage (MB) and the peak GPU memory usage (MB).

## 348 **B.6.2** Additional Results

The detailed time and space consumption of the node-level GC methods on *ogbn-arxiv* (0.50%) and graph-level GC methods on *ogbg-molhiv* (1 Graph/Cls) are shown in Table B13 and Table B14 respectively. For node-level methods, although trajectory matching methods (*SFGC* [42], *GEOM* [40]) may consume less time and memory due to their offline matching mechanism, the expert trajectories generated before matching can occupy up to 764 GB of space as shown in Table B15, significantly impacting storage requirements. Among all the graph-level GC methods, *Mirage* [9] stands out by not relying on any GPU resources for calculation and can condense data extremely quickly, taking only 1% of the time required by other methods.

Table D15. This and memory consumption of unrefert methods on <i>Ogon-arxiv</i> (0.507	Table B1	3: Time and	l memory consu	imption of	different	methods or	n ogbn-arxiv	(0.50%
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Consumption	GCDM	DM	DosCond	GCond	SGDD	SFGC	GEOM
Time (min)	212.90	57.70	117.38	266.57	226.62	245.65	148.37
Acc. (%)	58.09	58.09	60.73	61.28	61.51	67.13	67.29
CPU Memory (MB)	2720.88	2708.70	5372.60	5270.70	5426.30	3075.30	3335.10
GPU Memory (MB)	2719.74	2552.63	3850.24	3850.24	8326.35	4050.12	5308.42

356

## 357 C Reproducibility and Limitations

Accessibility and license. All the datasets, algorithm implementations, and experimental settings are publicly available in our open project (https://github.com/RingBDStack/GC-Bench). Our package (codes and datasets) is licensed under the MIT License. This license permits users to freely use, copy, modify, merge, publish, distribute, sublicense, and sell copies of the software, provided

Table B14: Time and memory consumption of different methods on *ogbg-molhiv* (1 Graph/Cls).

	augeen			
Consumption	DosCond	KiDD	Mirage	Citese
Time (min)	218.11	202.38	2.91	129
Acc. (%)	67.41	66.44	71.09	<b>EI</b> ! 1
CPU Memory (MB)	2666.29	3660.79	752.22	<b>F</b> IICK
GPU Memory (MB)	1005.98	6776.42	0.00	21

Table B15: Expert trajectory size (GB) for trajectory matching methods.

Citeseer	Cora	ogbn-arxiv	
129	152	15	
Flickr	Reddit	ACM	DBLP
21	42	312	764

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**Datasets.** *Cora, Citeseer, Flickr, Reddit* and *DBLP* are publicly available online<sup>1</sup> with the MIT license. *ogbn-arxiv, ogbg-molbace, ogbg-molbbp* and *ogbg-molhiv* are released by OGB [11] with the MIT license. *ACM* [41] is the subset hosted in [32] with the MIT license. *NCII* [29] and *DD* [3] are available in TU Datasets [25] with the MIT license. All the datasets are consented to by the authors for academic usage. All the datasets do not contain personally identifiable information or offensive content.

Limitations. GC-Bench has some limitations that we aim to address in future work. Our current 372 benchmark is limited to a specific set of graph types and graph tasks and might not reflect the full 373 potential and versatility of GC methods. We hope to implement more GC algorithms for various tasks 374 (e.g. subgraph classification, community detection) on more types of graphs (e.g., dynamic graph, 375 directed graph). Besides, due to resource constraints and the availability of implementations, we 376 could not include some of the latest GC algorithms in our benchmark. We will continuously update 377 our repository to keep track of the latest advances in the field. We are also open to any suggestions 378 and contributions that will improve the usability and effectiveness of our benchmark, ensuring it 379 remains a valuable resource for the IGL research community. 380

## 381 **References**

- [1] Michaël Defferrard, Xavier Bresson, and Pierre Vandergheynst. Convolutional neural networks on graphs
   with fast localized spectral filtering. *arXiv: Learning,arXiv: Learning*, 2016.
- [2] Kaize Ding, Jundong Li, Rohit Bhanushali, and Huan Liu. *Deep Anomaly Detection on Attributed Networks*,
   page 594–602. May 2019.
- [3] Paul D Dobson and Andrew J Doig. Distinguishing enzyme structures from non-enzymes without
   alignments. *Journal of molecular biology*, 2003.
- Junfeng Fang, Xinglin Li, Yongduo Sui, Yuan Gao, Guibin Zhang, Kun Wang, Xiang Wang, and Xiangnan
   He. Exgc: Bridging efficiency and explainability in graph condensation. *arXiv preprint arXiv:2402.05962*, 2024.
- [5] Matthias Fey and Jan Eric Lenssen. Fast graph representation learning with pytorch geometric. *arXiv* preprint arXiv:1903.02428, 2019.
- [6] Tao-yang Fu, Wang-Chien Lee, and Zhen Lei. Hin2vec: Explore meta-paths in heterogeneous information
   networks for representation learning. In *CIKM*, pages 1797–1806, 2017.
- [7] Jian Gao and Jianshe Wu. Multiple sparse graphs condensation. *Knowledge-Based Systems*, 278:110904,
   2023.
- [8] Xinyi Gao, Tong Chen, Yilong Zang, Wentao Zhang, Quoc Viet Hung Nguyen, Kai Zheng, and Hongzhi
   Yin. Graph condensation for inductive node representation learning. In *ICDE*, 2024.
- [9] Mridul Gupta, Sahil Manchanda, Sayan Ranu, and Hariprasad Kodamana. Mirage: Model-agnostic graph
   distillation for graph classification. In *ICLR*, 2024.
- [10] William L. Hamilton, Zhitao Ying, and Jure Leskovec. Inductive representation learning on large graphs.
   In *NeurIPS*, 2017.

<sup>1</sup>https://github.com/pyg-team/pytorch\_geometric

- [11] Weihua Hu, Matthias Fey, Marinka Zitnik, Yuxiao Dong, Hongyu Ren, Bowen Liu, Michele Catasta, and
   Jure Leskovec. Open graph benchmark: Datasets for machine learning on graphs. In *NeurIPS*, 2020.
- [12] Wei Jin, Xianfeng Tang, Haoming Jiang, Zheng Li, Danqing Zhang, Jiliang Tang, and Bing Yin. Condensing
   graphs via one-step gradient matching. In *SIGKDD*, 2022.
- [13] Wei Jin, Lingxiao Zhao, Shi-Chang Zhang, Yozen Liu, Jiliang Tang, and Neil Shah. Graph condensation
   for graph neural networks. In *ICLR*, 2021.
- [14] Thomas N Kipf and Max Welling. Semi-supervised classification with graph convolutional networks.
   *arXiv preprint arXiv:1609.02907*, 2016.
- [15] Thomas N Kipf and Max Welling. Variational graph auto-encoders. *arXiv preprint arXiv:1611.07308*,
   2016.
- [16] Johannes Klicpera, Aleksandar Bojchevski, and Stephan Günnemann. Predict then propagate: Graph
   neural networks meet personalized pagerank. In *ICLR*, 2018.
- [17] Xinglin Li, Kun Wang, Hanhui Deng, Yuxuan Liang, and Di Wu. Attend who is weak: Enhancing graph
   condensation via cross-free adversarial training. *arXiv preprint arXiv:2311.15772*, 2023.
- [18] Mengyang Liu, Shanchuan Li, Xinshi Chen, and Le Song. Graph condensation via receptive field
   distribution matching. *arXiv preprint arXiv:2206.13697*, 2022.
- 419 [19] Yang Liu, Deyu Bo, and Chuan Shi. Graph condensation via eigenbasis matching. In *ICML*, 2024.
- Yilun Liu, Ruihong Qiu, and Zi Huang. Cat: Balanced continual graph learning with graph condensation.
   In *ICDM*, pages 1157–1162. IEEE, 2023.
- Yilun Liu, Ruihong Qiu, and Zi Huang. Gcondenser: Benchmarking graph condensation. *arXiv preprint arXiv:2405.14246*, 2024.
- 424 [22] Yilun Liu, Ruihong Qiu, Yanran Tang, Hongzhi Yin, and Zi Huang. Puma: Efficient continual graph 425 learning with graph condensation. *arXiv preprint arXiv:2312.14439*, 2023.
- [23] Qingsong Lv, Ming Ding, Qiang Liu, Yuxiang Chen, Wenzheng Feng, Siming He, Chang Zhou, Jianguo
   Jiang, Yuxiao Dong, and Jie Tang. Are we really making much progress?: Revisiting, benchmarking and
   refining heterogeneous graph neural networks. In *SIGKDD*, 2021.
- Runze Mao, Wenqi Fan, and Qing Li. Gcare: Mitigating subgroup unfairness in graph condensation
   through adversarial regularization. *Applied Sciences*, 13(16):9166, 2023.
- [25] ChristopherJ. Morris, NilsM. Kriege, Franka Bause, Kristian Kersting, Petra Mutzel, and Marion Neumann.
   Tudataset: A collection of benchmark datasets for learning with graphs. *arXiv: Learning, arXiv: Learning*, Jul 2020.
- 434 [26] Qiying Pan, Ruofan Wu, Tengfei Liu, Tianyi Zhang, Yifei Zhu, and Weiqiang Wang. Fedgkd: Unleashing
   435 the power of collaboration in federated graph neural networks. *arXiv preprint arXiv:2309.09517*, 2023.
- 436 [27] Ozan Sener and Silvio Savarese. Active learning for convolutional neural networks: A core-set approach.
   437 In *ICLR*, 2018.
- Yunsheng Shi, Zhengjie Huang, Shikun Feng, Hui Zhong, Wenjin Wang, and Yu Sun. Masked label
   prediction: Unified message passing model for semi-supervised classification, 2021.
- [29] Nikil Wale, Ian A Watson, and George Karypis. Comparison of descriptor spaces for chemical compound
   retrieval and classification. *Knowledge and Information Systems*, 2008.
- [30] Chun Wang, Shirui Pan, Ruiqi Hu, Guodong Long, Jing Jiang, and Chengqi Zhang. Attributed graph
   clustering: A deep attentional embedding approach. In *IJCAI*, 2019.
- Lin Wang, Wenqi Fan, Jiatong Li, Yao Ma, and Qing Li. Fast graph condensation with structure-based
   neural tangent kernel. In *The Web Conference*, 2024.
- [32] Xiao Wang, Houye Ji, Chuan Shi, Bai Wang, Yanfang Ye, Peng Cui, and Philip S Yu. Heterogeneous graph
   attention network. In *The Web Conference*, 2019.
- 448 [33] Max Welling. Herding dynamical weights to learn. In *ICML*, pages 1121–1128, 2009.

- Felix Wu, Tianyi Zhang, AmauriH. Souza, Christopher Fifty, Tao Yu, and KilianQ. Weinberger. Simplifying
   graph convolutional networks. *arXiv: Learning,arXiv: Learning*, 2019.
- [35] Keyulu Xu, Weihua Hu, Jure Leskovec, and Stefanie Jegelka. How powerful are graph neural networks?
   In *ICLR*, 2018.
- [36] Zhe Xu, Yuzhong Chen, Menghai Pan, Huiyuan Chen, Mahashweta Das, Hao Yang, and Hanghang Tong.
   Kernel ridge regression-based graph dataset distillation. In *SIGKDD*, pages 2850–2861, 2023.
- [37] Beining Yang, Kai Wang, Qingyun Sun, Cheng Ji, Xingcheng Fu, Hao Tang, Yang You, and Jianxin Li.
   Does graph distillation see like vision dataset counterpart? In *NeurIPS*, 2023.
- [38] Hanqing Zeng, Hongkuan Zhou, Ajitesh Srivastava, Rajgopal Kannan, and Viktor K. Prasanna. Graphsaint:
   Graph sampling based inductive learning method. In *ICLR*, 2020.
- [39] Tianle Zhang, Yuchen Zhang, Kun Wang, Kai Wang, Beining Yang, Kaipeng Zhang, Wenqi Shao, Ping
   Liu, Joey Tianyi Zhou, and Yang You. Two trades is not baffled: Condense graph via crafting rational
   gradient matching. *arXiv preprint arXiv:2402.04924*, 2024.
- [40] Yuchen Zhang, Tianle Zhang, Kai Wang, Ziyao Guo, Yuxuan Liang, Xavier Bresson, Wei Jin, and Yang
   You. Navigating complexity: Toward lossless graph condensation via expanding window matching. *CoRR*,
   abs/2402.05011, 2024.
- [41] Jianan Zhao, Xiao Wang, Chuan Shi, Zekuan Liu, and Yanfang Ye. Network schema preserving heteroge neous information network embedding. In *IJCAI*, 2020.
- 467 [42] Xin Zheng, Miao Zhang, Chunyang Chen, Quoc Viet Hung Nguyen, Xingquan Zhu, and Shirui Pan.
- 468 Structure-free graph condensation: From large-scale graphs to condensed graph-free data. In *NeurIPS*, 2023.